The fish bioconcentration factor gold standard database: practical examples

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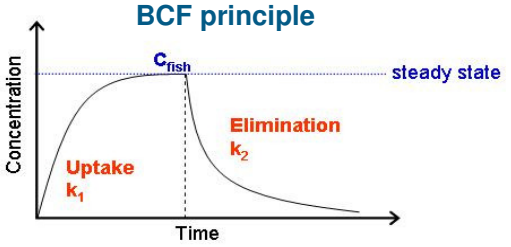
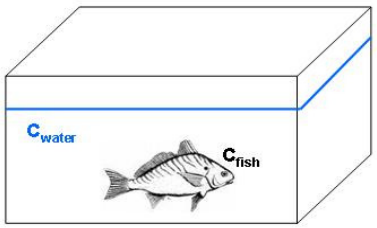
Introduction and Aims

The classical approach to derive BCF values (OECD 305 bioconcentration test) is labour intensive, costly and requires a lot of test animals. A database containing only high quality data was lacking. Within the LRI Eco7 project, a fish bioconcentration factor (BCF) 'gold standard database' has been developed and linked with the relational database Ambit for further (Q)SAR and alternative testing development. Criteria for considering substances as not bioaccumulative (i.e. unlikely to have a BCF > 2,000 (B) or 5000 (vB)) are mainly based on weight of evidence approaches and expert judgement, using parameters such as molecular length, Kow and molecular diameter. The validity of the following criteria was investigated using data from the fish BCF gold standard database in Ambit: (1) average diameter and molecular weight, (2) maximum molecular length, (3) log Kow.

BCF principle

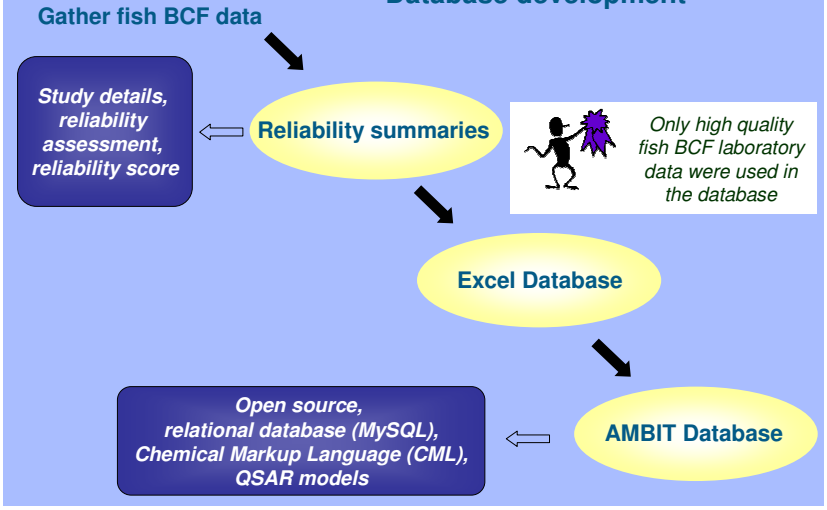




$$BCF_{ss} = \frac{C_{fish}}{C_{water}}$$

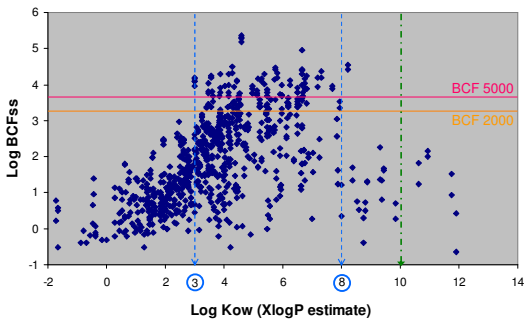
at steady state

Database development

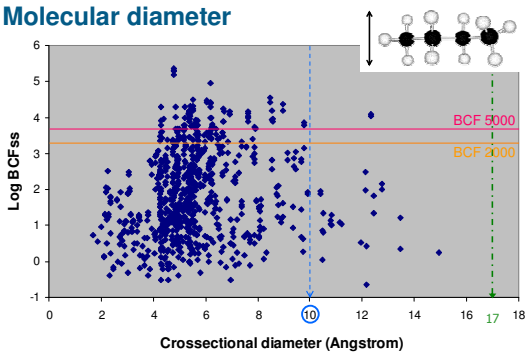


Bioaccumulation threshold criteria

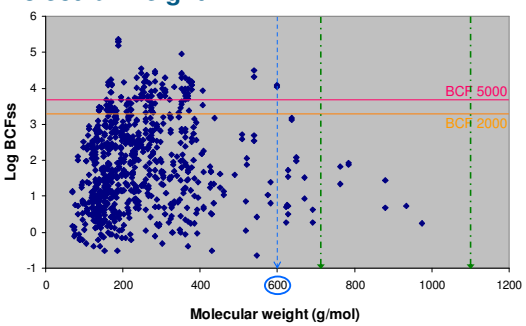
Log Kow



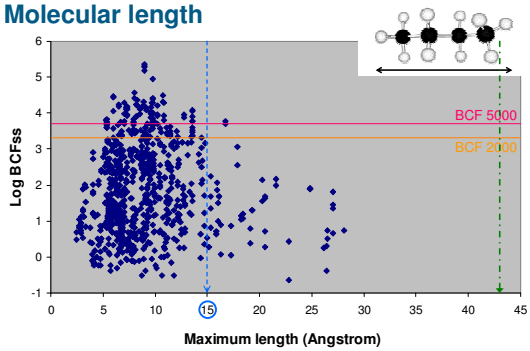
Molecular diameter



Molecular weight



Molecular length

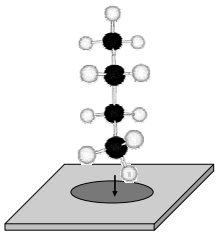


Cut-off levels observed by the authors

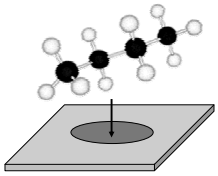
Cut-off levels established by the TECNES working group on PBTs

Effect of molecular size on uptake

Appropriate orientation



Inappropriate orientation



Conclusions

- Cut-off levels for considering substances as not bioaccumulative (i.e. unlikely to have a BCF > 2000 (B) or 5000 (vB)) are (1) log Kow < 3 or > 8, (2) molecular weight > 600 g/mol, (3) molecular diameter > 10 Å, (4) molecular length > 15 Å.
- Only a very limited number of substances had an 'unexpectedly' high BCF, e.g. highly chlorinated compounds such as hexachlorobenzene or heptachlorononorbornene.
- Results of the project are made publicly available as an easily accessible relational database (more info on http://www.euras.be/bcf). This database is embedded into the Ambit format (http://ambit.acad.bg).

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